METHODS IN THE QUANTUM THEORY OF MAGNETISM

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Sergei Vladimirovich Tyablikov was born in 1921 near Moscow. He studied at the physics department of the Moscow State University, where he continued his postgraduate studies. In 1946 he obtained a Candidate's degree, and in 1954 was awarded his doctorate. Currently, Dr. Tyablikov is a Professor of Theoretical and Mathematical Physics.

Professor Tyablikov's interests range over theoretical solid state physics, the theory of polarons, and the quantum theories of magnetism. He has published about 70 papers and was the author, with Professor V. L. Bonch-Bruevich, of "Green's Function Method in Statistical Mechanics" (Fizmatgiz, Moscow, 1961). Since 1947, Professor Tyablikov has worked at the V. A. Steklov Mathematical Institute of the Academy of Sciences of the USSR, and is now chairman of the department of statistical mechanics.

The original Russian text was published by Nauka Press in Moscow in 1965.

СЕРГЕЙ ВЛАДИМИРОВИЧ ТЯБЛИКОВ

МЕТОДЫ КВАНТОВОЙ ТЕОРИИ МАГНЕТИЗМА

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METHODS IN THE QUANTUM THEORY OF MAGNETISM

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METHODS IN THE QUANTUM THEORY OF MAGNETISM

Foreword

Only rarely does one find translations from Russian of scientific material that read as if they had originally been written in English. Mr. Tybulewicz has achieved this objective and is to be commended for it.

The present monograph will appeal to the students of magnetism and others who appreciated the Green function methods previously introduced by Bonch-Bruevich and Tyablikov,* but who felt that the sections on magnetism in the earlier book were too compact. Much the same material is discussed here, but in a much more leisurely manner than heretofore. Tyablikov might well have entitled the present monograph "Theories of the Heisenberg Model," for he treats this model from many points of view: (a) ground state properties (ferromagnetic, antiferromagnetic, helical, etc.), (b) dynamics and quantum mechanics, and (c) thermodynamical and statistical properties. Concepts of spin-wave theory, molecular-field theory, ferromagnetic resonance, and of Bogolyubov's "method of approximate second-quantization" are developed in the present context well before the Green function theory is even introduced. Some recent developments, such as H.B. Callen's improved decoupling scheme, are described, and, in general, the text covers many of the interesting applications of the formalism to cooperative magnetism.

It is only fair to point out that two important areas of research have been omitted entirely, namely, the origins of the magnetic interaction (e.g., superexchange, Hund's rules, etc.), and

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*V. L. Bonch-Bruevich and S. V. Tyablikov "Green's Function Method in Statistical Mechanics" North-Holland Publ. Co., Amsterdam, 1962.

the band theory of magnetism (i.e., the magnetism of iron,nickel, and similar transition metals). English-speaking readers can satisfy their curiosity as to where the Heisenberg Hamiltonian finds its ultimate justification, or about where it is not valid, in several texts or reviews* where these subjects are adequately covered. But it is only here, in Tyablikov's monograph, that one finds an authoritative statement of recent Soviet work in the mathematical theory of the Heisenberg model of magnetism.

New York
September 1966

D.C. Mattis

*G.T. Rado and H. Suhl, Eds. "Magnetism" Academic Press, New York; in several volumes, 1963 and following.
D. Mattis "The Theory of Magnetism" Harper & Row, New York, 1965.

Preface to the American Edition

The theory of magnetic phenomena in solids is being rapidly developed by many investigators in a number of countries. Obviously, it is well nigh impossible to write a book in which the results are right up to date. The present book has a more modest aim – to acquaint the reader with some of the fundamental methods in the quantum theory of magnetism; it does not pretend to give a complete account of all the methods or the results obtained by these methods. It is hoped that the book will be found useful by English-language readers.

S. V. Tyablikov

May 1966

Preface

Magnetic properties are exhibited to a greater or lesser extent by all substances. Among solids, we can distinguish a group of magnetic substances whose magnetic properties are particularly pronounced: ferromagnets, ferrimagnets, and antiferromagnets. The present treatment deals with some of the problems arising in the theory of the magnetic phenomena in such substances. We shall call the theory of phenomena in strongly magnetic substances the theory of strong magnetism or, simply, the theory of magnetism, because the weakly magnetic substances (paramagnets and diamagnets) will not be considered. The emphasis is on the methods giving general solutions and on the features characteristic of magnetic problems. The microscopic approach is used throughout.

Considerable progress has been made in recent years in the investigation of the many-body problem. The progress is, to a considerable extent, due to the application of quantum-field methods to statistical mechanics. Consequently, there has also been progress in the quantum theory of magnetism. However, the results of many interesting investigations have not yet been presented systematically. This creates certain difficulties for those who are new to the theory of magnetism, with its problems and methods of solution.

In this book, the author attempts to present, from a single standpoint, some of the methods used in the quantum theory of magnetism. The primary aim is to present systematically the theoretical apparatus in a form which would allow the reader to use it in investigations of still unsolved problems. The book also includes some additional topics in order to save the reader the trouble of referring to other sources, some of which may not be very accessible. The treatment does not pretend to be a comprehensive review of all the results obtained in the quantum theory of magnetism. It simply presents one of the directions of development pursued recently both in the Soviet Union and abroad.

The first part of the book (Chaps. I–III) is methodological in its approach. It begins with a brief introduction, in which the basic topics and definitions of the physics of magnetic phenomena and the elements of the phenomenological theory are presented. The second quantization method is described, the problem of spin Hamiltonians in the theory of strong magnetism is dealt with, and the essentials of statistical mechanics are presented briefly.

In the second part (Chaps. IV–VIII), the approximate second quantization (spin-wave) method (Chaps. IV–V), the molecular field method, elements of the perturbation theory at high temperatures (Chap. VI), and the method of Green's quantum functions (Chaps. VII–VIII) are presented.

This organization of the material makes it possible to consider systematically the calculation methods for low and high temperatures (including the vicinity of the Curie point), as well as the interpolation methods covering the whole range of temperatures. The general theories are presented first and the necessary mathematical apparatus is developed; this is followed by applications. The applications of a method are demonstrated by a more or less detailed analysis of one or two very simple problems in the theory of magnetism. Other applications are reviewed briefly at the ends of the chapters dealing with the applications of the methods. The applications referred to do not cover even a small part of the numerous results in the theory of magnetism, since this was not the purpose of the present monograph. In most cases, only those investigations are mentioned which are to some extent related to the problems discussed in the book. The exception is made for some theoretical problems which, in the opinion of the author, are of interest but which are not treated in the book because of lack of space.

The discussions always refer to single-crystal one-domain samples. To avoid repetition, this will not be mentioned again.

The system of units with $\hbar = 1$ is employed throughout the book.

The appendices contain information on the reciprocal lattice space, the formal Fourier transformations for a discrete medium, and problems associated with them.

The book is mainly intended for those who wish to become familiar with the elements of the quantum theory of magnetism and methods used in this theory, as well as postgraduate students and senior undergraduates. It is assumed that the reader is already familiar with the fundamentals of quantum and statistical mechanics as presented in the standard courses given by physics departments of universities and institutes of higher learning.

The book was read in manuscript by A.A. Gusev, A. G. Gurevich, and V.A. Moskalenko, to whom the author is grateful for their numerous comments and advice. He would also like to record his thanks to his colleagues for sending him preprints of their papers, which enabled him to become acquainted with a number of interesting results before their publication.

The author is grateful to Academician N.N. Bogolyubov for his valuable contribution to discussions of various problems in the quantum theory of magnetism and for reading the manuscript.

S. V. Tyablikov

List of Principal Symbols

$\mathcal{A}_1, \mathcal{A}_2, \ldots$	– one-particle, two-particle, etc., operators
$C, C(\ldots, n_f, \ldots)$	– wave function in the second quantization representation
$E_\nu, E(\nu)$	– energy of an elementary excitation
$\mathcal{E}, \mathcal{E}_n$	– energy of a system
F	– free energy
F_s	– distribution function of s particles
$G, G^{(j)}, \mathcal{G}$	– Green's quantum functions
H	– constant magnetic field
$H_\ominus$	– demagnetizing field
H_c	– critical field
$\mathcal{H}$	– Hamiltonian of a system
I, I_1	– exchange integral for nearest neighbors
$I(f_1, f_2)$	– exchange integral for atoms at sites f_1 and f_2
$I(\omega)$	– spectral density or spectral function
$J(\nu)$	– Fourier transform of the exchange integral $I(f)$
K_i, K_i'	– i-th anisotropy constants
M	– magnetization of a sample
M_0	– saturation magnetization
$M_1, M(E)$	– mass operator for the first Green's function
$\mathcal{M}$	– magnetic moment operator of a system
N	– number of atoms in a lattice, number of particles in a system
$N_{\alpha\beta}$	– demagnetization factor tensor
$\bar{N}_\nu$	– average value of the number of particles (occupation number) in a state ν
$\mathcal{N}$	– operator for the total number of particles
$\mathcal{N}_\nu, n_\nu$	– operator for the number of particles in a state ν
P	– particle permutation operator, principal value symbol

$\mathcal{P}$ – projection operator
Q – partition function
S_f^{α} – α-component of the spin at a site f
S_f, S – value of the spin at a site f
S^{α} – operator for the total spin of a system
T – temperature
T_C – Curie temperature
T_N – Néel temperature
T_k – compensation temperature
V – volume of a system
$Z_p(x)$ – modified Riemann's zeta function
b_f^+, b_f – Pauli operators
f, g – numbers of lattice sites, numbers of one-particle states
$h(t)$ – alternating magnetic field
k – Boltzmann's constant
$\overline{m}$ – average magnetization per site
t – time
v – volume per site or per particle
z – number of nearest neighbors
Γ – damping of elementary excitations
γ^{α} – direction cosines of the magnetization vector
$\Delta(\nu_1 - \nu_2)$, δ_{ν_1, ν_2} – Kronecker's delta
δ – vector joining two nearest neighbors
$\delta(x)$ – Dirac's delta function
$\zeta(p)$ – Riemann's zeta function
ϑ – temperature in units of k
ϑ_C – Curie temperature
ϑ_N – Néel temperature
λ – chemical potential
μ, μ_f – magnetic moment of an atom; magnetic moment of an atom in units of S, S_f
μ_B – Bohr magneton
ν, $\varkappa$ – wave vector
ρ – density matrix
ρ_s – density matrix for a system of s particles
σ_s, σ_s^{α} – relative magnetization
τ – dimensionless temperature
τ_C – dimensionless Curie temperature
χ – susceptibility
Ω – thermodynamic potential

Contents

Chapter I

Introduction

In this chapter, we present general information and definitions relating to the theory of strong magnetism, and review briefly the theoretical ideas about the nature of strong magnetism. On this basis, we give a qualitative classification of the main types of magnetic substance.

Sec. 1. General Information and Definitions *

According to their magnetic properties, solids can be divided into weakly magnetic (diamagnetic and paramagnetic) and strongly magnetic (ferromagnetic, antiferromagnetic, and ferrimagnetic). Our treatment will deal only with the theoretical problems involving strongly magnetic substances.

* For detailed treatments of experimental data and theoretical problems relating to ferromagnetism, see the monographs of Akulov (1939), Vonsovskii and Shur (1948), Bogolyubov (1949), Belov (1951, 1959), Vonsovskii (1952), Bozorth (1956), Landau and Lifshits (1959), Gurevich (1960), and various collections: "Physics of Ferromagnetic Domains" (1951), "Ferromagnetic Resonance" (1952), "Magnetic Structure of Ferromagnets" (1959), "Ferromagnetic Resonance" (1961), "Theory of the Ferromagnetism of Metals and Alloys" (1963); for antiferromagnetism, see also the reviews of Nagamiya et al. (1955), Borovik–Romanov (1962), Belov et al. (1964), and "Antiferromagnetism" (1956); for weak ferromagnetism, see a review by Borovik–Romanov (1962) and a monograph by Turov (1963); for ferrimagnetism, see the reviews of Gorter (1955), Pakhomov and Smol'kov (1962), and a monograph by Smit and Wijn (1962).

Ferromagnets, antiferromagnets, and ferrimagnets are characterized by the existence, under certain conditions, of magnetic ordering and large macroscopic moments due to this ordering (such moments always appear in ferromagnets and ferrimagnets). The order of magnitude of these macroscopic moments is $N\mu_B$, where N is the number of atoms in a sample and μ_B is the Bohr magneton.

Transition metals (iron, cobalt, nickel) are typical ferromagnets; transition-metal oxides and other salts (FeO, CoO, CoF_2, $NiSO_4$, etc.), are typical antiferromagnets; typical ferrimagnets are compounds of transition elements in the form of complex salts ($MnO \cdot Fe_2O_3$, $3Y_2O_3 \cdot 5Fe_2O_3$, etc.) and some other compounds.

According to current ideas, the magnetism of solids is due to the electrons of partly filled inner shells of atoms. The strong magnetism appears only in those cases when the crystal lattice of a substance includes atoms with partly filled inner shells.

Partly filled inner shells are found in elements of the transition groups of iron (3d-shell), palladium (4d-shell), platinum (5d-shell), actinium (6d- and 5f - shells), as well as rare-earth elements (4f - shell). Table 1 gives the electron configurations of the partly filled shells, and of the shells next to them, for all these elements. The presence of atoms with partly filled inner shells is not a sufficient condition for the existence of strong magnetism.

Thus, in the iron group (3d-metals), pure Sc, Ti, and V are paramagnetic, Cr and Mn are antiferromagnetic, and Fe, Co, and Ni are ferromagnetic.

In the palladium group (4d-metals), Y, Zr, Nb, Mo, Tc, Ru, and Rh are all paramagnetic and the problem of the magnetic properties of Pd is not solved yet [according to Abragams (1963), this metal is not antiferromagnetic].

In the platinum group (5d-metals), La, Lu, Hf, Ta, W, Re, Os, and Ir are paramagnetic, while Pt is antiferromagnetic.

In the rare-earth group (4f - metals), some elements exist in two different magnetic phases at low temperatures. In the subgroup containing Ce, Pr, Nd, Pm, Sm, and Eu, antiferromagnet-

Table 1. Electron Configurations in Partly Filled Shells and in Shells which Follow Them, for Transition Elements in the Periodic System*

Iron group (electron configurations outside the Ar shell)

Sc	Ti	V	Cr	Mn	Fe	Co	Ni
$3d^{1}4s^{2}$	$3d^{2}4s^{2}$	$3d^{3}4s^{2}$	$3d^{5}4s$	$3d^{5}4s^{2}$	$3d^{6}4s^{2}$	$3d^{7}4s^{2}$	$3d^{8}4s^{2}$

Palladium group (electron configurations outside the Kr shell)

Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd
$4d^{1}5s^{2}$	$4d^{2}5s^{2}$	$4d^{4}5s$	$4d^{5}5s$	$4d^{5}5s^{2}$	$4d^{7}5s$	$4d^{8}5s$	$4d^{10}$

Platinum group (electron configurations outside the Xe shell for La and outside the Xe + $4f^{14}$ shell for remaining elements)

La							
$5d^{1}6s^{2}$							
Lu	Hf	Ta	W	Re	Os	Ir	Pt
$5d^{1}6s^{2}$	$5d^{2}6s^{2}$	$5d^{3}6s^{2}$	$5d^{4}6s^{2}$	$5d^{5}6s^{2}$	$5d^{6}6s^{2}$	$5d^{7}6s^{2}$	$5d^{9}6s$

Rare-earth elements (electron configurations outside the Xe shell)

Ce	Pr	Nd	Pm	Sm	Eu	Gd
$4f^{2}6s^{2}$	$4f^{3}6s^{2}$	$4f^{4}6s^{2}$	$4f^{5}6s^{2}$	$4f^{6}6s^{2}$	$4f^{7}6s^{2}$	$4f^{7}5d^{1}6s^{2}$

Tb	Dy	Ho	Er	Tm	Yb
$4f^{8}5d^{1}6s^{2}$	$4f^{10}6s^{2}$	$4f^{11}6s^{2}$	$4f^{12}6s^{2}$	$4f^{13}6s^{2}$	$4f^{14}6s^{2}$